Spin dynamics in the regime of hopping conductivity

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We consider spin dynamics in the impurity band of a semiconductor with spin-split spectrum. Due to the splitting, phonon-assisted hops from one impurity to another are accompanied by rotation of the electron spin, which leads to spin relaxation. The system is strongly inhomogeneous because of exponential variation of hopping times. However, at very small couplings an electron diffuses over a distance exceeding the characteristic scale of the inhomogeneity during the time of spin relaxation, so one can introduce an averaged spin relaxation rate. At larger values of coupling the system is effectively divided into two subsystems: the one where relaxation is very fast and another one where relaxation is rather slow. In this case, spin decays due to escape of the electrons from one subsystem to another. As a result, the spin dynamics is non-exponential and hardly depends on spin-orbit coupling.

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Spin dynamics in semiconductors has attracted much attention in the last decades (for review, see Ref. [1]). A great number of publications were devoted to the study of the spin relaxation in the metallic regime, where it is usually dominated by the Dyakonov-Perel mechanism. According to this mechanism, the spin relaxation rate is proportional to the diffusion coefficient [2]. Recently, the idea was put forward [3] that this proportionality goes beyond the metallic regime and stays valid in the regime of hopping conductivity:

$$1/\tau_S^{(1)} \sim D/L_S^2$$
. (1)

Here $\tau_S^{(1)}$ is the spin relaxation time, $L_S \sim v/\Omega$, v is the tunnelling velocity, and Ω is the typical value of spin precession frequency for an electron moving under the barrier.

In this paper we discuss spin dynamics in the hopping regime and show that a number of spin relaxation mechanisms are realized in addition to the one discussed in Ref. [3]. The hopping regime takes place at small temperatures $T \ll W$ (here W is the width of the impurity band). In the opposite limit $T \gg W$ the transport is governed by activation to the mobility edge. However, methodologically it is convenient to start from the modelling case when $T \gg W$ but transitions to the conduction band are forbidden. This model is rather simple because the probability of a hop does not depend on temperature. On the other hand, it captures basic physics of the problem and can be easily generalized to the real situation. We neglect electron-electron interaction and assume that the distance between impurities is much larger than the Bohr radius a: $na^d \ll 1$ (here n is the impurity concentration). We also assume that $L_S \gg a$ which is usually the case.

Due to the spin-orbit coupling, phonon-assisted hops are accompanied by rotation of the electron spin. The rotation angle can be written as $\varphi = \varphi_0 + \delta \varphi$, where φ_0 corresponds to the quasiclassical approximation, which im-

plies that electron moves under barrier along the straight line connecting the impurities and $\delta \varphi$ is the correction which is due to quantum uncertainty of the trajectory (this correction cannot be neglected when we consider non-typical hops over the distances of the order of several a). The angle φ_0 is given by $\varphi_0 = \Omega(\mathbf{v})t$, where $\Omega(\mathbf{v})$ is proportional to spin-orbit spectrum splitting, $\mathbf{v} = \mathbf{n}\hbar/ma$ is the tunnelling velocity, t = r/v, a is the Bohr radius, m is the electron mass, r is the hopping length, and **n** is the unit vector in the direction of the hop. In the 3D case $\Omega_x \sim v_x(v_y^2 - v_z^2)$ and the other components are given by cyclical transmutations [4]. In the 2D case $\Omega = \mathbf{a}v_x + \mathbf{b}v_y$, where constant vectors **a** and **b** depend on the quantum well orientation and the degree of asymmetry of the confining potential [5, 6]. The characteristic value of φ_0 is given by

$$\varphi_0 \sim r/L_S.$$
 (2)

Random hops between impurities lead to spin relaxation. Let us assume that at t=0 the homogeneous distribution of the spin density \mathbf{S}_0 is created in the system (for example, by means of optical orientation) and study the dynamics of the averaged spin density $\mathbf{S}(t)$. The system under discussion is strongly inhomogeneous due to exponential variation of hopping times. Indeed, the waiting time τ_{ij} of a hop between impurities i and j varies exponentially with the distance L_{ij} between impurities: $\tau_{ij} = \tau_0 \exp(2L_{ij}/a)$, where τ_0 is the waiting time for the impurities separated by the distance of the order of a (here we took into account that $T \gg W$). We assume [7] that impurities i and j are effectively connected if $\tau_{ij} < t$, or, equivalently,

$$L_{ij} < L(t) = a/2 \ln(t/\tau_0),$$

and disconnected if $\tau_{ij} > t$ $(L_{ij} > L(t))$. For L(t) larger than a certain critical length $L_h \sim n^{-1/d}$, the connected impurities form infinite cluster. The fraction of impurities $P(\xi)$ belonging to the infinite cluster increases with

increasing of t as shown in Fig.1. Here

$$\xi = \xi(t) = L(t)/L_h = (a/2L_h)\ln(t/\tau_0). \tag{3}$$

Near the critical point $(L(t) = L_h)$ the share of impurities belonging to the infinite cluster P behaves as a power function: $P = (\xi - 1)^{\beta}$, (where β is critical index), and with the further increase of ξ it is quickly saturated [7].

The exponential regime of the spin relaxation $\mathbf{S}(t) = \mathbf{S}_0 \exp(-t/\tau_S)$ with an averaged rate $1/\tau_S$ is realized at sufficiently small spin-orbit coupling, when an electron has enough time to visit almost any possible impurity configuration during the time τ_S . This condition is satisfied when

$$1 - P[\xi(\tau_S)] \ll 1. \tag{4}$$

There are two contributions to $1/\tau_S$. The first one is due to electron diffusion on the scales larger than the scale of inhomogeneity. This contribution is given by Eq. (1) [3]. Another contribution, neglected in Ref. [3], comes from the spin relaxation on non-typical clusters with the distances between impurities on the order of several a. The most likely non-typical configurations of impurities are pairs and triangles. An electron captured on a non-typical complex makes many hops in a small region of space before it leaves it. The shift in space due to these hops is limited by the size of the complex, while the deviation of its spin increases with the number of hops. Therefore, such complexes do not contribute to the diffusion process but they might give essential contribution to the spin relaxation.

The most probable non-typical configuration is a pair of impurities. In quasi-classical approximation the contribution of pairs to spin relaxation is equal to zero, because the rotation of the spin during the hop from one impurity to another is compensated by the rotation during the hope in the opposite direction. However, when the distance between impurities is of the order of a, the deviation of the trajectory from the quasi-classical one due to quantum uncertainty is of the order of the size of the quasiclassical trajectory itself. This implies that the correction $\delta \varphi$ to the rotation angle is comparable with φ_0 (i.e. $\delta \varphi \sim \varphi_0 \sim a/L_S \ll 1$). This is indeed the case in 3D semiconductors. In the 2D case the situation is more subtle. In this case the rotation angle in the first order of $1/L_S$ depends only on the shift of the electron in space $\varphi = \int \Omega dt = \mathbf{a} r_x + \mathbf{b} r_y$ (here the integration is taken over the electron trajectory and we took into account that small rotations commute) and does not depend on a particular trajectory. As a result, the correction to the main contribution appears only in the next orders in $1/L_S$: $\delta \varphi \sim (a/L_S)^m$, where $m \geq 2$. One can show that m=2 for the components of the spin which are perpendicular to $[\mathbf{a} \times \mathbf{b}]$ and m = 3 for the parallel component. The exact value of this correction depends on the wave vector of the phonon that was emitted or absorbed during the hop [8]. Therefore, the rotation angle is a random quantity.

In general case, the angle of the rotation after passing the closed trajectory (that includes the hop from the first impurity to the second one and the hop in the opposite direction) can be written as:

$$\delta \varphi \sim (a/L_S)^m,$$
 (5)

where m = 1 in 3D case and m = 2, 3 in 2D case.

After rotation by the angle $\delta\varphi$, spin projection on the original direction decreases on the average by $\delta\varphi^2$. So, one can expect that a relaxation rate on a single pair is given by $(a/L_S)^{2m}(1/\tau_0)$. However, this estimate does not take into account the effects of level repulsion. The repulsion energy is on the order of $\Delta E \sim (e^2/\kappa a)e^{-r/a}$. A non-typical pair can participate in the spin relaxation only if $\Delta E \leq T$. Therefore, the minimal distance between impurities in a non-typical pair is given by $r^* \geq a \ln(\kappa a/Te^2)$. The hop waiting time for such a pair is given by $\tau_0 \exp(2r^*/a) \sim \tau_0 (e^2/T\kappa a)^2$, this leads to an additional factor $(T\kappa a/e^2)^2 \ll 1$ in the spin relaxation rate. As a result, the rate of the spin relaxation on a single non-typical pair reads

$$1/\tau_S^* \sim (a/L_S)^{2m} (1/\tau_0) (T\kappa a/e^2)^2$$
. (6)

The contribution of non-typical pairs to the spin relaxation rate is proportional to $1/\tau_S^*$ and to the share of the time that electron spends on non-typical pairs. This share is proportional to the ratio of the concentration of non-typical pairs n^* to the total impurity concentration: $n^*/n \sim (a/L_h)^d$. Hence, the corresponding relaxation rate is given by

$$1/\tau_S^{(2)} \sim (a/L_h)^d (a/L_S)^{2m} (1/\tau_0) (T\kappa a/e^2)^2.$$
 (7)

Both mechanisms described above are additive and the spin relaxation rate is:

$$1/\tau_S = 1/\tau_S^{(1)} + 1/\tau_S^{(2)}. (8)$$

Let us compare these two mechanisms. In the case under discussion, when $T\gg W$, the diffusion coefficient entering Eq. (1) is determined by the hops over the critical length: $D\sim \exp(-2L_h/a)$ [7]. Therefore, $1/\tau_S^{(1)}$ decreases exponentially with the average distance between impurities, while $1/\tau_S^{(2)}$ decreases according to slow power law $1/L_h^d$ (see Eq. (7)). In the 3D case the dependence on L_S in Eq. (7) is the same as in Eq. (1). Therefore, in the 3D case, $1/\tau_S^{(2)}\gg 1/\tau_S^{(1)}$ (since we assumed that $L_h\gg a$). In the 2D case, $1/\tau_S^{(2)}$ decreases with L_S faster than $1/\tau_S^{(1)}$. Thus, at very small spinorbit coupling the main contribution is given by Eq. (1). However, the crossover to the regime of non-typical pairs takes place already at exponentially small value of the coupling.

In deriving Eq. (7) we assumed that during the process of spin relaxation an electron has enough time to visit many non-typical pairs which are separated by a distance on the order of $[n^*]^{-1/d} = L_h(L_h/a)$ (this is the length that plays the role of inhomogeneity scale in this regime). With the increasing of the strength of spin-orbit coupling this condition fails because spin relaxation time decreases and there appear finite clusters that are effectively separated from the rest of the system on the time scale on the order of τ_S . Since the concentration of nontypical pairs n^* is small, most of the isolated clusters do not contain them. This means that the spin of electrons captured on the isolated clusters does not relax until they escape to the infinite cluster where the relaxation is much faster (it is still determined by Eq. (8)). Therefore, the infinite cluster can be considered as a "black hole" for electron spin. The spin dynamics in this regime is given

$$\mathbf{S}(t) = \mathbf{S}_0[1 - P(t)],\tag{9}$$

where $P(t) = P[L(t)/L_h] = P[(a/2L_h) \ln(t/\tau_0)]$. Hence, the spin polarization is a function of a single dimensionless parameter $(a/2L_h) \ln(t/\tau_0)$. It worth noting that the dynamics of the spin relaxation in this regime does not depend on the strength of spin-orbit coupling.

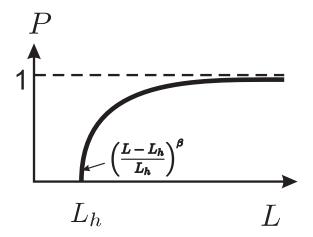


FIG. 1: Fraction of impurities belonging to the infinite cluster as a function of the maximal distance L between connected impurities. In the vicinity of the critical length L_h , function $P[L/L_h]$ increases as $[L/L_h-1]^{\beta}$, where β is a critical index.

With the further increase of the coupling, the spin relaxation on the finite clusters comes into play. Finally, at extremely high coupling the spin rotates by a large angle after one typical hop. In this case, the spin relaxes on any finite clusters except isolated impurities separated from the rest of the system by distances larger than L(t). The spin at the moment t is proportional to the number

of electrons captured on such "traps":

$$\mathbf{S}(t) = \mathbf{S}_0 \exp \left[-C_d \left(\frac{a}{L_h} \ln \frac{t}{\tau_0} \right)^d \right], \tag{10}$$

where d=2,3 is dimensionality of the system and $C_d \sim 1$ is a numerical coefficient. It is seen from this equation that just as in the case of intermediate coupling the spin dynamics does not depend on the spin-orbit strength and determined by the only parameter $(a/L_h) \ln(t/\tau_0)$.

Next, we discuss qualitatively the generalization of the approach discussed above to the case of small temperatures. In this case the waiting time is given by $\tau_{ij} = \tau_0 \exp(L_{ij}/a + E_{ij}/T)$, where E_{ij} is the energy difference between states i and j. The minimization of this exponent yields the optimal values of hopping length $L_{ij} \sim L_h(T)$ and hopping energy $E_{ij} \sim E_h(T)$ which are given by [7]:

$$\frac{E_h(T)}{T} \sim \frac{L_h(T)}{a} \sim (gTa^d)^{-1/(d+1)}$$
 (11)

(these equations are applicable when $T < Wa/L_h$). The optimal length $L_h(T)$ is of the order of the average distance between impurities lying in the energy band of width $E_h(T)$ (optimal energy band). The states outside the band of width $E_h(T)$ near the Fermi level are not accessible to polarized electrons. As a consequence, the equations derived above are still valid with two modifications. First, one should make a replacement $L_h \to L_h(T)$. Second, the effective dimension of the system should be increased $d \to d+1$, which takes into account the motion of the electron along energy axis.

To conclude, the theory of the spin relaxation of the electrons in the impurity band was developed and a number of different relaxation regimes were predicted. At weak spin-orbit couplings spin relaxation is exponential with the rate of spin relaxation given by two contributions: the first one comes from the relaxation on non-typical pairs of impurities and the second one is due to electron diffusion on the scales larger than the scale of inhomogeneity of the system. At stronger couplings, spin relaxation is due to escapes of the electrons from finite clusters to the infinite one. In this case, the law of spin relaxation does not depend on the spin-orbit coupling. At very large couplings the spin relaxation is due to escape from the spin traps.

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- [8] The rigorous approach to the derivation of $\delta\varphi$ implies calculation of the matrix element that describes phonon-assisted hop from one impurity to another. Such calculation shows that in the limit $qa \leq 1$ (where \mathbf{q} is the phonon wave-vector), that is most relevant in the realistic semi-conductor structures, the characteristic value of $\delta\varphi$ does not depend on the parameter qa, but depends on the direction of the vector \mathbf{q} .